

Full wwPDB X-ray Structure Validation Report (i)

Sep 10, 2023 - 05:23 PM EDT

:	4JDJ
:	Crystal structure of Serine/threonine-protein kinase PAK 4 F461V mutant in
	complex with Paktide T peptide substrate
:	Ha, B.H.; Boggon, T.J.
	2013-02-25
:	2.30 Å(reported)
	: : :

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org A user guide is available at https://www.wwpdb.org/validation/2017/XrayValidationReportHelp with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

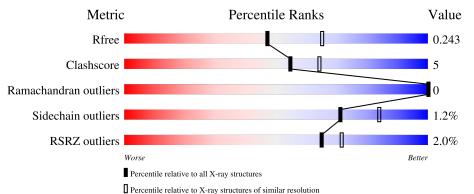
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	$\begin{array}{c} \textbf{Whole archive} \\ (\#\textbf{Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length		Quality of chain							
1	А	346	.%	75% 9% · 16%							
2	В	15	20%	27%	7%	60%	_				



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2479 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a protein called Serine/threenine-protein kinase PAK 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	А	290	Total 2311	C 1470	N 406	0 419	Р 2	S 14	0	4	0

Chain	Residue	Modelled	Actual	Comment	Reference
А	246	MET	-	expression tag	UNP O96013
А	247	GLY	-	expression tag	UNP 096013
А	248	SER	-	expression tag	UNP 096013
А	249	SER	-	expression tag	UNP O96013
А	250	HIS	-	expression tag	UNP 096013
А	251	HIS	-	expression tag	UNP 096013
А	252	HIS	-	expression tag	UNP 096013
А	253	HIS	-	expression tag	UNP 096013
А	254	HIS	-	expression tag	UNP 096013
А	255	HIS	-	expression tag	UNP 096013
А	256	SER	-	expression tag	UNP O96013
А	257	SER	-	expression tag	UNP 096013
А	258	GLY	-	expression tag	UNP 096013
А	259	LEU	-	expression tag	UNP O96013
А	260	VAL	-	expression tag	UNP O96013
А	261	PRO	-	expression tag	UNP 096013
А	262	ARG	-	expression tag	UNP O96013
А	263	GLY	-	expression tag	UNP 096013
А	264	SER	-	expression tag	UNP 096013
А	265	HIS	-	expression tag	UNP O96013
А	266	MET	-	expression tag	UNP 096013
А	267	GLU	-	expression tag	UNP O96013
А	268	ASN	-	expression tag	UNP O96013
А	269	LEU	-	expression tag	UNP 096013
А	270	TYR	-	expression tag	UNP 096013
А	271	PHE	-	expression tag	UNP 096013
А	272	GLN	-	expression tag	UNP 096013

There are 41 discrepancies between the modelled and reference sequences:

Continued on next page...



Chain	Residue	Modelled	Actual	Comment	Reference
А	273	GLY	-	expression tag	UNP O96013
А	274	ALA	-	expression tag	UNP O96013
А	275	ARG	-	expression tag	UNP O96013
А	276	ALA	-	expression tag	UNP O96013
А	277	ARG	-	expression tag	UNP O96013
А	278	GLN	-	expression tag	UNP O96013
А	279	GLU	-	expression tag	UNP O96013
А	280	ASN	-	expression tag	UNP O96013
A	281	GLY	-	expression tag	UNP O96013
А	282	MET	-	expression tag	UNP O96013
А	283	PRO	-	expression tag	UNP O96013
А	284	GLU	-	expression tag	UNP O96013
А	285	LYS	-	expression tag	UNP O96013
А	461	VAL	PHE	engineered mutation	UNP O96013

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• Molecule 2 is a protein called Paktide T.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	В	6	Total 66	C 42	N 16	0 8	0	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	А	102	Total (102 10))2	0	0





3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Chain A: $\frac{1}{100}$
- \bullet Molecule 1: Serine/threonine-protein kinase PAK 4



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants	61.79Å 61.79Å 181.73Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 - 2.30	Depositor
Resolution (A)	45.43 - 2.30	EDS
% Data completeness	100.0 (50.00-2.30)	Depositor
(in resolution range)	$100.0 \ (45.43 - 2.30)$	EDS
R _{merge}	0.09	Depositor
R _{sym}	0.09	Depositor
$< I/\sigma(I) > 1$	$1.55 (at 2.29 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
D D.	0.195 , 0.244	Depositor
R, R_{free}	0.195 , 0.243	DCC
R_{free} test set	835 reflections $(5.08%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	36.2	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.34, 31.3	EDS
L-test for twinning ²	$ < L >=0.48, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2479	wwPDB-VP
Average B, all atoms $(Å^2)$	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.93% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, TPO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 5 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bo	nd lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.46	1/2344~(0.0%)	0.58	0/3172	
2	В	0.97	1/68~(1.5%)	0.65	0/90	
All	All	0.49	2/2412~(0.1%)	0.58	0/3262	

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	В	1	TRP	CD2-CE2	5.50	1.48	1.41
1	А	392	TRP	CD2-CE2	5.18	1.47	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	А	2311	0	2372	22	1
2	В	66	0	67	5	0
3	А	102	0	0	2	0
All	All	2479	0	2439	25	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.



Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
1:A:319:SER:O	1:A:341:ARG:NH2	2.19	0.76
1:A:337[B]:ILE:HD11	1:A:346:LEU:HD13	1.78	0.66
1:A:332:THR:HG21	3:A:690:HOH:O	1.96	0.64
1:A:411:ARG:HA	1:A:411:ARG:HE	1.63	0.62
1:A:411:ARG:HA	1:A:411:ARG:NE	2.16	0.59
1:A:311:VAL:HG13	1:A:367:VAL:HG11	1.86	0.57
1:A:528:ARG:O	1:A:555:ARG:NH2	2.35	0.57
2:B:-3:ARG:NH1	2:B:-2:ARG:H	2.04	0.54
1:A:518:GLU:HG3	1:A:526:MET:HE1	1.90	0.53
1:A:332:THR:HG23	2:B:2:TYR:OH	2.10	0.51
1:A:411:ARG:HE	1:A:411:ARG:CA	2.25	0.49
1:A:308:LEU:HD12	1:A:354:LEU:HD21	1.99	0.45
2:B:-1:ARG:HH11	2:B:-1:ARG:HB3	1.81	0.44
1:A:322:ASP:OD2	1:A:341:ARG:HD3	2.18	0.43
1:A:521:LEU:HD23	1:A:524:MET:HE1	2.00	0.43
1:A:432:HIS:CG	1:A:494:PRO:HB3	2.53	0.43
1:A:332:THR:HB	1:A:352:MET:HG2	2.01	0.42
1:A:562:TPO:O2P	1:A:564:ALA:HB3	2.18	0.42
1:A:413:ASN:HB2	3:A:603:HOH:O	2.19	0.42
1:A:521:LEU:HA	1:A:524:MET:HE3	2.01	0.42
1:A:518:GLU:HG3	1:A:526:MET:CE	2.49	0.41
2:B:-1:ARG:HB3	2:B:-1:ARG:NH1	2.36	0.41
1:A:411:ARG:NE	1:A:411:ARG:CA	2.84	0.41
1:A:545:LEU:HD13	1:A:571:PHE:CZ	2.56	0.41
1:A:477:GLY:O	2:B:1:TRP:N	2.49	0.40

All (25) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:GLU:OE2	1:A:489:ARG:NH1[7_545]	2.10	0.10

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries



of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	А	289/346~(84%)	283~(98%)	6(2%)	0	100	100
2	В	4/15~(27%)	4 (100%)	0	0	100	100
All	All	293/361~(81%)	287~(98%)	6(2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	254/299~(85%)	251~(99%)	3~(1%)	71 84
2	В	6/10~(60%)	6 (100%)	0	100 100
All	All	260/309~(84%)	257~(99%)	3~(1%)	71 84

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	332	THR
1	А	410	THR
1	А	444	ASP

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. There are no such side chains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.



5.4 Non-standard residues in protein, DNA, RNA chains (i)

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with |Z| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Turne	Chain	Dec	Tinle	Link Bond lengths			Bond angles		
IVIOI	Type	Chain	Res	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
1	TPO	А	562	1	8,10,11	1.11	1 (12%)	10,14,16	0.96	0
1	SEP	А	474	1	8,9,10	0.64	0	8,12,14	1.28	1 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	А	562	1	-	2/9/11/13	-
1	SEP	А	474	1	-	0/5/8/10	-

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	А	562	TPO	P-OG1	2.56	1.64	1.59

All (1) bond length outliers are listed below:

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	474	SEP	O3P-P-O2P	2.12	115.73	107.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	А	562	TPO	CB-OG1-P-O2P
1	А	562	TPO	O-C-CA-CB



There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	А	562	TPO	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ $>$	#RSRZ>2	$OWAB(Å^2)$	$Q{<}0.9$
1	А	288/346~(83%)	-0.26	3 (1%) 82 86	25, 37, 59, 78	1 (0%)
2	В	6/15~(40%)	2.56	3 (50%) 0 0	55, 72, 84, 88	0
All	All	294/361~(81%)	-0.20	6 (2%) 65 71	25, 37, 62, 88	1 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	2	TYR	7.7
1	А	331	SER	3.8
2	В	1	TRP	3.6
2	В	-1	ARG	3.0
1	А	521	LEU	2.4
1	А	519	PRO	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{\AA}^2)$	Q < 0.9
1	TPO	А	562	11/12	0.89	0.15	$35,\!38,\!45,\!45$	4
1	SEP	А	474	10/11	0.99	0.09	30,33,35,36	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.



6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

